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Microcanonical Ensemble and Algebra of Conserved Generators for Generalized Quantum Dynamics

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Abstract : It has recently been shown, by application of statistical mechanical methods to determine the canonical ensemble governing the equilibrium distribution of operator initial values, that complex quantum field theory can emerge as a statistical approximation to an underlying generalized quantum dynamics. This result was obtained by an argument based on a Ward identity analogous to the equipartition theorem of classical statistical mechanics. We construct here a microcanonical ensemble which forms the basis of this canonical ensemble. This construction enables us to define the microcanonical entropy and free energy of the field configuration of the equilibrium distribution and to study the stability of the canonical ensemble. We also study the algebraic structure of the conserved generators from which the microcanonical and canonical ensembles are constructed, and the flows they induce on the phase space.

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1. Introduction

Generalized quantum dynamics[1,2] is an analytic mechanics on a symplectic set of operator valued variables, forming an operator valued phase space $\mathcal{S}$. These variables are defined as the set of linear transformations† on an underlying real, complex, or quaternionic Hilbert space (Hilbert module), for which the postulates of a real, complex, or quaternionic quantum mechanics are satisfied[2−6]. The dynamical (generalized Heisenberg) evolution, or flow, of this phase space is generated by the total trace Hamiltonian $\mathbf{H} = \mathbf{Tr}H$, where for any operator O we have

$$\begin{aligned}\mathbf{O} \equiv \mathbf{Tr}\mathrm{O} &\equiv \mathrm{ReTr}(-1)^F \mathrm{O} \\ &= \mathrm{Re}\sum_n \langle n|(-1)^F \mathrm{O}|n\rangle,\end{aligned} \tag{1.1}$$

H is a function of the operators $\{q_r(t)\}, \{p_r(t)\}, \quad \mathrm{r} = 1, 2, \ldots, N$ (realized as a sum of monomials, or a limit of a sequence of such sums; in the general case of local noncommuting fields, the index r contains continuous variables), and $(-1)^F$ is a grading operator with eigenvalue $1(-1)$ for states in the boson (fermion) sector of the Hilbert space. Operators are called bosonic or fermionic in type if they commute or anticommute, respectively, with $(-1)^F$; for each r, p_r and q_r are of the same type.

The derivative of a total trace functional with respect to some operator variation is defined with the help of the cyclic property of the **Tr** operation. The variation of any monomial O consists of terms of the form $\mathrm{O}_L \delta x_r \mathrm{O}_R$, for x_r one of the $\{q_r\}, \{p_r\}$, which, under the **Tr** operation, can be brought to the form

$$\delta \mathbf{O} = \delta \mathbf{Tr}\mathrm{O} = \pm \mathbf{Tr}\mathrm{O}_R \mathrm{O}_L \delta x_r,$$

so that sums and limits of sums of such monomials permit the construction of

$$\delta \mathbf{O} = \mathbf{Tr}\sum_r \frac{\delta \mathbf{O}}{\delta x_r}\delta x_r, \tag{1.2}$$

uniquely defining $\delta\mathbf{O}/\delta x_r$.

Assuming the existence of a total trace Lagrangian[1,2] $\mathbf{L} = \mathbf{L}(\{q_r\}, \{\dot{q}_r\})$, the variation of the total trace action

$$\mathbf{S} = \int_{-\infty}^{\infty} \mathbf{L}(\{q_r\}, \{\dot{q}_r\})dt \tag{1.3}$$

results in the operator Euler-Lagrange equations

$$\frac{\delta \mathbf{L}}{\delta q_r} - \frac{d}{dt}\frac{\delta \mathbf{L}}{\delta \dot{q}_r} = 0. \tag{1.4}$$

As in classical mechanics, the total trace Hamiltonian is defined as a Legendre transform,

$$\mathbf{H} = \mathbf{Tr}\sum_r p_r \dot{q}_r - \mathbf{L}, \tag{1.5}$$

† In general, local (noncommuting) quantum fields.

where

$$p_r = \frac{\delta \mathbf{L}}{\delta \dot{q}_r}. \tag{1.6}$$

It then follows from (1.4) that

$$\frac{\delta \mathbf{H}}{\delta q_r} = -\dot{p}_r \qquad \frac{\delta \mathbf{H}}{\delta p_r} = \epsilon_r \dot{q}_r, \tag{1.7}$$

where $\epsilon_r = 1(-1)$ according to whether p_r, q_r are of bosonic (fermionic) type.

Defining the generalized Poisson bracket

$$\{\mathbf{A}, \mathbf{B}\} = \mathbf{Tr} \sum_r \epsilon_r \left(\frac{\delta \mathbf{A}}{\delta q_r} \frac{\delta \mathbf{B}}{\delta p_r} - \frac{\delta \mathbf{B}}{\delta q_r} \frac{\delta \mathbf{A}}{\delta p_r} \right), \tag{1.8a}$$

one sees that

$$\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + \{\mathbf{A}, \mathbf{H}\}. \tag{1.8b}$$

Conversely, if we define

$$\mathbf{x}_s(\eta) = \mathbf{Tr}(\eta x_s), \tag{1.9a}$$

for η an arbitrary, constant operator (of the same type as x_s, which denotes here q_s or p_s), then

$$\frac{d\mathbf{x}_s(\eta)}{dt} = \mathbf{Tr} \sum_r \epsilon_r \left(\frac{\delta \mathbf{x}_s(\eta)}{\delta q_r} \frac{\delta \mathbf{H}}{\delta p_r} - \frac{\delta \mathbf{H}}{\delta q_r} \frac{\delta \mathbf{x}_s(\eta)}{\delta p_r} \right), \tag{1.9b}$$

and comparing the coefficients of η on both sides, one obtains the Hamilton equations (1.7) as a consequence of the Poisson bracket relation (1.8b).

The Jacobi identity is satisfied by the Poisson bracket of (1.8a),[7] and hence the total trace functionals have many of the properties of the corresponding quantities in classical mechanics.[8] In particular, canonical transformations take the form

$$\delta \mathbf{x}_s(\eta) = \{\mathbf{x}_s(\eta), \mathbf{G}\}, \tag{1.10a}$$

which implies that

$$\delta p_r = -\frac{\delta \mathbf{G}}{\delta q_r}\ , \quad \delta q_r = \epsilon_r \frac{\delta \mathbf{G}}{\delta p_r}\ , \tag{1.10b}$$

with the generator $\mathbf{G}$ any total trace functional constructed from the operator phase space variables. Time evolution then corresponds to the special case $\mathbf{G} = \mathbf{H}dt$.

It has recently been shown by Adler and Millard[9] that a canonical ensemble can be constructed on the phase space $\mathcal{S}$, reflecting the equilibrium properties of a system of many degrees of freedom. Since the operator

$$\begin{aligned} \tilde{C} &= \sum_r (\epsilon_r q_r p_r - p_r q_r) \\ &= \sum_{r,B} [q_r, p_r] - \sum_{r,F} \{q_r, p_r\}, \end{aligned} \tag{1.11}$$

where the sums are over bosonic and fermionic pairs, respectively, is conserved under the evolution (1.7) induced by the total trace Hamiltonian, the canonical ensemble must be constructed taking this constraint into account. This is done by constructing the conserved quantity $\mathbf{Tr}\tilde{\lambda}\tilde{C}$, for some given constant anti-hermitian operator $\tilde{\lambda}$.

In the general case, in the presence of the fermionic sector, the graded trace of the Hamiltonian is not bounded from below, and the partition function may be divergent. When the equations of motion induced by the Lagrangian $\mathbf{L}$ coincide with those induced by the ungraded total trace of the same Lagrangian,

$$\hat{\mathbf{L}} = \mathrm{Re}\mathrm{Tr}L,$$

without the factor $(-1)^F$, the corresponding ungraded total trace Hamiltonian $\hat{\mathbf{H}}$ is conserved; it may therefore be included as a constraint functional in the canonical ensemble, along with the new conserved quantity $\hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}$ (see Appendices 0 and C of ref. 9), where

$$\begin{aligned}\hat{\tilde{C}} &= \sum_r [q_r, p_r] \\ &= \sum_{r,B} [q_r, p_r] + \sum_{r,F} [q_r, p_r].\end{aligned} \tag{1.12}$$

It was argued that the Ward identities derived from the canonical ensemble imply that $\hat{\tilde{\lambda}}$ and $\tilde{\lambda}$ are functionally related, so that they may be diagonalized in the same basis (Appendix F of ref. 9). It was then shown that, since the ensemble averages depend only on $\tilde{\lambda}$ and $(-1)^F$, the ensemble average of any operator must commute with these operators. Since the ensemble averaged operator $\langle\tilde{C}\rangle_{AV}$ is anti-self-adjoint, if one furthermore assumes it is completely degenerate (with eigenvalue $i_{eff}\hbar$), the ensemble average of the theory then reduces to the usual complex quantum field theory. In this paper, we construct a microcanonical ensemble from which the canonical ensemble of ref. 9 can be obtained following the usual methods of statistical mechanics. This construction gives some insight into the interpretation of the parameters, relates the canonical and microcanonical entropies, and identitifies the generalized free energy. It also permits estimates of the statistical fluctuations admitted by the canonical ensemble, and error bounds on the Ward identity which we shall treat elsewhere. We give, in this framework, a self-consistency proof of the stability of the canonical ensemble. We then go on to discuss the algebraic structure of the canonical generators related to the conserved operators $\tilde{C}$ and $\hat{\tilde{C}}$, and the flows on phase space induced by these generators.

2. The microcanonical and canonical ensembles

Introducing a complete set of states $\{|n\rangle\}$ in the underlying Hilbert space, the phase space operators are completely characterized by their matrix elements $\langle m|x_r|n\rangle \equiv (x_r)_{mn}$, which have the form

$$(x_r)_{mn} = \sum_A (x_r)^A_{mn} e_A, \tag{2.1}$$

where A takes the values 0, 1 for complex Hilbert space, 0, 1, 2, 3 for quaternion Hilbert space (technically, a Hilbert module), and just the one value 0 for real Hilbert space, and the e_A are the associated hypercomplex units (unity, complex, or quaternionic units[2]). The mathematical procedures we establish here are applicable to more general Hilbert modules; arguments are given in ref. 2, however, for restricting our attention to these three cases, and we shall therefore concentrate on the real, complex, and quaternionic structures in the examination of specific properties. The phase space measure is then defined as

$$\begin{aligned} d\mu &= \prod_A d\mu^A, \\ d\mu^A &\equiv \prod_{r,m,n} d(x_r)^A_{mn}, \end{aligned} \tag{2.2}$$

where redundant factors are omitted according to adjointness conditions. The measure defined in this way is invariant under canonical transformations induced by the generalized Poisson bracket.[9]

We then define the microcanonical ensemble in terms of the set of states in the underlying Hilbert space which satisfy δ-function constraints on the values of the two total trace functionals $\mathbf{H}$, $\hat{\mathbf{H}}$ and the matrix elements of the two conserved operator quantities $\tilde{C}$, $\hat{\tilde{C}}$ discussed in the previous section. The volume of the corresponding submanifold in phase space is given by

$$\begin{aligned} \Gamma(E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}) = \int & d\mu \, \delta(E - \mathbf{H}) \, \delta(\hat{E} - \hat{\mathbf{H}}) \\ & \prod_{n \leq m, A} \delta(\nu^A_{nm} - \langle n|(-1)^F \tilde{C}|m\rangle^A) \, \delta(\hat{\nu}^A_{nm} - \langle n|\hat{\tilde{C}}|m\rangle^A), \end{aligned} \tag{2.3}$$

where we have used the abbreviations $\tilde{\nu} \equiv \{\nu^A_{nm}\}$ and $\hat{\tilde{\nu}} \equiv \{\hat{\nu}^A_{nm}\}$ for the parameters in the arguments on the left hand side. The factor $(-1)^F$ in the term with $\tilde{C}$ is not essential, but convenient in obtaining the precise form given in ref. 9 for the canonical distribution. The entropy associated with this ensemble is given by

$$S_{mic}(E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}) = \log \Gamma(E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}). \tag{2.4}$$

As we shall see, it is not possible to associate a temperature to this structure in the usual simple way.

The operators $\tilde{C}$ and $\hat{\tilde{C}}$ are defined in terms of sums over degrees of freedom. In the context of the application to quantum field theory, the enumeration of degrees of freedom includes continuous parameters, corresponding to the measure space of the fields. These operators may therefore be decomposed into parts within a certain (large) region of the measure space, which we denote as b, corresponding to what we shall consider as a *bath*, in the sense of statistical mechanics, and within another (small) part of the measure space, which we denote as s, corresponding to what we shall consider as a *subsystem.* We shall assume that the functionals $\mathbf{H}$ and $\hat{\mathbf{H}}$ may also be decomposed additively into parts

associated with b and s; this assumption is equivalent to the presence of interactions in the Hamiltonian or Lagrangian operators which are reasonably localized in the measure space of the fields (the difference in structure between the Lagrangian and Hamiltonian consists of operators that are explicitly additive), so that the errors in assuming additivity are of the nature of "surface terms". The constraint parameters may then be considered to be approximately additive as well, and we may rewrite the microcanonical ensemble as

$$\begin{aligned}\Gamma(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}) = \int & d\mu_b\, d\mu_s\, dE_s\, d\hat{E}_s\, (d\nu^s)\, (d\hat{\nu}^s) \\ & \times \delta(E - E_s - \mathbf{H}_b)\,\delta(E_s - \mathbf{H}_s)\delta(\hat{E} - \hat{E}_s - \hat{\mathbf{H}}_b)\delta(\hat{E}_s - \hat{\mathbf{H}}_s) \\ & \times \prod_{n\le m, A} \delta(\nu^A_{nm} - \nu^{A,s}_{nm} - \langle n|(-1)^F \tilde{C}_b|m\rangle^A)\,\delta(\nu^{A,s}_{nm} - \langle n|(-1)^F \tilde{C}_s|m\rangle^A) \\ & \times \delta(\hat{\nu}^A_{nm} - \hat{\nu}^{A,s}_{nm} - \langle n|\hat{\tilde{C}}_b|m\rangle^A)\,\delta(\hat{\nu}^{A,s}_{nm} - \langle n|\hat{\tilde{C}}_s|m\rangle^A).\end{aligned} \tag{2.5}$$

We recognize the integrations over $d\mu_s$ and $d\mu_b$ in (2.5) in terms of the corresponding microcanonical subensembles, for the bath b and subsystem s respectively, i.e., we may write (2.5) as

$$\Gamma(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}}) = \int dE_s d\hat{E}_s (d\nu^s)(d\hat{\nu}^s)\,\Gamma_b(E - E_s, \hat{E} - \hat{E}_s, \tilde{\nu} - \tilde{\nu}_s, \hat{\tilde{\nu}} - \hat{\tilde{\nu}}_s)\,\Gamma_s(E_s, \hat{E}_s, \tilde{\nu}_s, \hat{\tilde{\nu}}_s). \tag{2.6}$$

We now assume that the integrand in (2.6) has a maximum, for a large number of degrees of freedom, that dominates the integral. In the treatment of the statistical mechanics of classical particles, the number of degrees of freedom generally vastly exceeds the number of variables controlling the constraint hypersurfaces in the phase space; in our case, due to the presence of the constraints imposed by the operators $\tilde{C}$ and $\hat{\tilde{C}}$, there are an infinite number of variables, and the question of the development of a significant maximum may be more delicate. We will demonstrate, however, that due to the semidefinite form of the autocorrelation matrix of the fluctuations, the canonical distribution that we obtain with this assumption is at least locally stable.

Let us, for brevity, define

$$\xi = \{\xi_i\} \equiv \{E, \hat{E}, \tilde{\nu}, \hat{\tilde{\nu}}\}, \tag{2.7}$$

where the index i refers to the elements of the set of variables, so that (2.6) takes the form

$$\Gamma(\Xi) = \int d\xi_s \Gamma_b(\Xi - \xi_s)\Gamma_s(\xi_s), \tag{2.8a}$$

where Ξ corresponds to the set of total properties for the whole ensemble. A necessary condition for an extremum in all of the variables at $\xi_s = \bar{\xi}$ is then

$$\frac{\partial}{\partial \xi}[\Gamma_b(\Xi - \xi)\Gamma_s(\xi)]|_{\bar{\xi}} = 0, \tag{2.8b}$$

which implies that

$$\frac{1}{\Gamma_s(\xi)}\frac{\partial\Gamma_s}{\partial\xi_i}(\xi)|_{\bar{\xi}} = \frac{1}{\Gamma_b(\Xi-\xi)}\frac{\partial\Gamma_b}{\partial\Xi_i}(\Xi-\xi)|_{\bar{\xi}}. \tag{2.8c}$$

The logarithmic derivatives in (2.8c) define a set of quantities analogous to the (reciprocal) temperature of the usual statistical mechanics, i.e., equilibrium-fixing Lagrange parameters common to the bath and the subsystem. We write these separately as

$$\begin{aligned}\tau &= \frac{\partial}{\partial E}\log\Gamma_s(\xi)|_{\bar{\xi}}\\ \hat{\tau} &= \frac{\partial}{\partial \hat{E}}\log\Gamma_s(\xi)|_{\bar{\xi}}\\ \lambda^A_{nm} &= -\frac{\partial}{\partial \nu^A_{nm}}\log\Gamma_s(\xi)|_{\bar{\xi}}\\ \hat{\lambda}^A_{nm} &= -\frac{\partial}{\partial \hat{\nu}^A_{nm}}\log\Gamma_s(\xi)|_{\bar{\xi}}.\end{aligned} \tag{2.9}$$

According to the definition of entropy (2.4), the bath phase space volume is given by

$$\begin{aligned}\Gamma_b(\Xi-\xi_s) &= e^{S_b(\Xi-\xi_s)}\\ &\cong e^{S_b(\Xi)}\exp\{-\sum_i \xi_{i,s}\frac{\partial S_b}{\partial\Xi_i}(\Xi)\},\end{aligned} \tag{2.10}$$

Neglecting the small shift in argument $\Xi \to \Xi - \xi_s$, it follows from (2.8$a-c$), (2.9), and (2.10) that

$$\Gamma_b(\Xi-\xi_s) \cong e^{S_b(\Xi)}\exp\{-\tau E_s - \hat{\tau}\hat{E}_s + \sum_{n\le m,A}(\nu^{A,s}_{nm}\lambda^A_{nm} + \hat{\nu}^{A,s}_{nm}\hat{\lambda}^A_{nm})\}. \tag{2.11}$$

We now return to (2.6), replacing the phase space volume of the bath, Γ_b, by the approximate form (2.11), and the subsystem phase space volume Γ_s by the phase space integral over the constraint δ-functions, i.e. (we use the equality henceforth, although it should be understood that we have included just the dominant contribution),

$$\begin{aligned}\Gamma(\Xi) = &\int d\mu_s dE_s d\hat{E}_s (d\nu^s)(d\hat{\nu}^s)\delta(E_s - \mathbf{H}_s)\delta(\hat{E}_s - \hat{\mathbf{H}}_s)\\ &\times \prod_{n\le m,A}\delta(\nu^{A,s}_{nm} - \langle n|(-1)^F\tilde{C}_s|m\rangle^A)\,\delta(\hat{\nu}^{A,s}_{nm} - \langle n|\hat{\tilde{C}}_s|m\rangle^A)\\ &\times e^{S_b(\Xi)}\exp\{-\tau E_s - \hat{\tau}\hat{E}_s + \sum_{n\le m,A}(\nu^{A,s}_{nm}\lambda^A_{nm} + \hat{\nu}^{A,s}_{nm}\hat{\lambda}^A_{nm})\}.\end{aligned} \tag{2.12}$$

Carrying out the integrals over the parameters, the δ-functions imply the replacement of the parameters E_s,$\hat{E}_s$, $\nu^{A,s}_{nm}$, $\hat{\nu}^{A,s}_{nm}$ in the exponent by the corresponding phase space quantities. For the product

$$\lambda^A_{nm}\langle n|(-1)^F\tilde{C}_s|m\rangle^A, \tag{2.13}$$

we note that the anti-self-adjoint property of $\tilde{C}_s$ implies that

$$\langle n|(-1)^F\tilde{C}_s|m\rangle = -\langle m|(-1)^F\tilde{C}_s|n\rangle^*, \tag{2.14}$$

with * denoting conjugation of the hypercomplex units, so that

$$\begin{aligned}\langle n|(-1)^F\tilde{C}_s|m\rangle^0 &= -\langle m|(-1)^F\tilde{C}_s|n\rangle^0,\\ \langle n|(-1)^F\tilde{C}_s|m\rangle^A &= \langle m|(-1)^F\tilde{C}_s|n\rangle^A, \quad A\neq 0,\end{aligned} \tag{2.15}$$

for all three cases of real, complex, or quaternionic Hilbert spaces. Thus we have

$$\mathrm{Re}\lambda_{nm}\langle m|(-1)^F\tilde{C}_s|n\rangle = -\sum_A \lambda_{nm}^A\langle n|(-1)^F\tilde{C}_s|m\rangle^A. \tag{2.16a}$$

Defining the operator $\tilde{\lambda}$ for which the matrix elements are

$$\begin{aligned}\langle n|\tilde{\lambda}|n\rangle^A =&\lambda_{nn}^A,\\ \langle n|\tilde{\lambda}|m\rangle^A =&\frac{1}{2}\lambda_{nm}^A, \quad n<m,\end{aligned} \tag{2.16b}$$

we see that the sum over $n\leq m$ of the expression (2.16a) is $\mathbf{Tr}\tilde{\lambda}\tilde{C}_s$. A similar result holds for the last term of (2.12) (in this case, since we did not insert the factor $(-1)^F$, we obtain the $\hat{\mathbf{Tr}}$ functional). The volume in phase space is then

$$\Gamma(\Xi) = e^{S_b(\Xi)}\int d\mu_s \exp -\{\tau\mathbf{H}_s + \hat{\tau}\hat{\mathbf{H}}_s + \mathbf{Tr}\tilde{\lambda}\tilde{C}_s + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}_s\}, \tag{2.17}$$

so that the normalized canonical distribution function (with the subscripts s removed) is given by

$$\rho = Z^{-1}\exp -\{\tau\mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}\}, \tag{2.18}$$

where

$$Z = \int d\mu \,\exp -\{\tau\mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{2.19}$$

This formula coincides with that obtained by Adler and Millard.[9] Note that the operators $\tilde{\lambda}$ and $\hat{\tilde{\lambda}}$ appear as an infinite set of inverse "temperatures", i.e., equilibrium Lagrange parameters associated both with the bath and the subsystem, corresponding to the conserved matrix elements of $(-1)^F\tilde{C}$ and $\hat{\tilde{C}}$.

We finally remark that the microcanonical entropy defined in (2.4) provides the Jacobian of the transformation from the integration over the measure of $\mathcal{S}$ in (2.19) to an integral over the parameters defining the microcanonical shells. To see this, we rewrite (2.19) as

$$\begin{aligned}Z = &\int d\mu dEd\hat{E}(d\nu)(d\hat{\nu})\delta(E-\mathbf{H})\,\delta(\hat{E}-\hat{\mathbf{H}})\\ &\times\prod_{n\leq m,A}\delta(\nu_{nm}^A - \langle n|(-1)^F\tilde{C}|m\rangle^A)\,\delta(\hat{\nu}_{nm}^A - \langle n|\hat{\tilde{C}}|m\rangle^A)\\ &\times\exp -\{\tau E + \hat{\tau}\hat{E} + \mathbf{Tr}\tilde{\lambda}\tilde{\nu} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{\nu}}\},\end{aligned} \tag{2.20a}$$

where we have defined the anti-self-adjoint parametric operators $\tilde{\nu}$ and $\hat{\tilde{\nu}}$ by

$$\begin{aligned}\nu^A_{nm} =&\langle n|(-1)^F\tilde{\nu}|m\rangle^A,\\ \hat{\nu}^A_{nm} =&\langle n|\hat{\tilde{\nu}}|m\rangle^A.\end{aligned} \tag{2.20b}$$

The phase space integration over the δ-function factors reproduces the volume of the microcanonical shell associated with these parameters, i.e, the exponential of the microcanonical entropy, so that the partition function can be written as

$$Z = \int dE d\hat{E}(d\nu)(d\hat{\nu})e^{S_{mic}(E,\hat{E},\tilde{\nu},\hat{\tilde{\nu}})}\exp -\{\tau E + \hat{\tau}\hat{E} + \mathbf{Tr}\tilde{\lambda}\tilde{\nu} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{\nu}}\}. \tag{2.21}$$

3. Stability and thermodynamic relations

In this section, we study the stability of the canonical ensemble as associated with the dominant contribution to the microcanonical phase space volume. To this end, we formally define the free energy A as the negative of the logarithm of the partition function,

$$Z \equiv e^{-A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})}, \tag{3.1}$$

so that (2.19) can be written as

$$1 = \int d\mu e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})}\exp -\{\tau\mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{3.2}$$

Differentiating with respect to[♯] τ, $\hat{\tau}$, and the matrix elements λ^A_{nm}, $\hat{\lambda}^A_{nm}$, we obtain (as in Eqs. (49) of ref. 9)

$$\frac{\partial A}{\partial \tau} = \langle \mathbf{H}\rangle_{AV}, \tag{3.3}$$

$$\frac{\partial A}{\partial \hat{\tau}} = \langle \hat{\mathbf{H}}\rangle_{AV}, \tag{3.4}$$

and using

$$\begin{aligned}\mathbf{Tr}\tilde{\lambda}\tilde{C} =& -\sum_{n\le m,A}\lambda^A_{nm}\langle n|(-1)^F\tilde{C}|m\rangle^A,\\ \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}} =& -\sum_{n\le m,A}\hat{\lambda}^A_{nm}\langle n|\hat{\tilde{C}}|m\rangle^A,\end{aligned} \tag{3.5}$$

we find

$$\frac{\partial A}{\partial \lambda^A_{nm}} = -\langle\langle n|(-1)^F\tilde{C}|m\rangle^A\rangle_{AV} \equiv -\langle C^A_{nm}\rangle_{AV}, \tag{3.6}$$

[♯] The hypercomplex index A should not be confused with the conventional symbol for the free energy.

$$\frac{\partial A}{\partial \hat{\lambda}^A_{nm}} = -\langle\langle n|\hat{C}|m\rangle^A\rangle_{AV} \equiv -\langle \hat{C}^A_{nm}\rangle_{AV}. \tag{3.7}$$

We now consider the identity

$$0 = \int d\mu\, (\mathbf{H} - \langle \mathbf{H}\rangle_{AV}) e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})} \exp -\{\tau\mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{3.8}$$

Differentiating with respect to τ, one finds

$$\begin{aligned} 0 = \int d\mu\, \big(\frac{\partial A}{\partial \tau} - \mathbf{H}\big)(\mathbf{H} - \langle \mathbf{H}\rangle_{AV}) e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})} \\ \times \exp -\{\tau\mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}\} - \frac{\partial \langle \mathbf{H}\rangle_{AV}}{\partial \tau}, \end{aligned} \tag{3.9}$$

so that, from (3.3), we find that (as in ref. 9)

$$\langle (\mathbf{H} - \langle \mathbf{H}\rangle_{AV})^2\rangle_{AV} = -\frac{\partial \langle \mathbf{H}\rangle_{AV}}{\partial \tau} = -\frac{\partial^2 A}{\partial \tau^2} \geq 0. \tag{3.10}$$

In fact, applying this argument to all of the parameters, we now show that A is a locally convex function. With this result, we will prove the stability of the canonical ensemble.

The derivative of (3.8) with respect to $\hat{\tau}$ yields, using the second of (3.3),

$$\langle (\mathbf{H} - \langle \mathbf{H}\rangle_{AV})(\hat{\mathbf{H}} - \langle \hat{\mathbf{H}}\rangle_{AV}) = -\frac{\partial \langle \mathbf{H}\rangle_{AV}}{\partial \hat{\tau}} = -\frac{\partial^2 A}{\partial \tau \partial \hat{\tau}}. \tag{3.11}$$

In the same way that we obtained (3.10), we also find (using $\hat{\mathbf{H}} - \langle \hat{\mathbf{H}}\rangle_{AV}$ as a factor in the integrand),

$$\langle (\hat{\mathbf{H}} - \langle \hat{\mathbf{H}}\rangle_{AV})^2\rangle_{AV} = -\frac{\partial \langle \hat{\mathbf{H}}\rangle_{AV}}{\partial \hat{\tau}} = -\frac{\partial^2 A}{\partial \hat{\tau}^2} \geq 0. \tag{3.12}$$

We consider next the identity

$$0 = \int d\mu\, (C^A_{nm} - \langle C^A_{nm}\rangle_{AV}) e^{A(\tau,\hat{\tau},\tilde{\lambda},\hat{\tilde{\lambda}})} \exp -\{\tau\mathbf{H} + \hat{\tau}\hat{\mathbf{H}} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}\}. \tag{3.13}$$

Differentiating with respect to $\lambda^B_{n'm'}$ and $\hat{\lambda}^B_{n'm'}$, we find

$$\begin{aligned} \frac{\partial^2 A}{\partial \lambda^A_{nm} \partial \lambda^B_{n'm'}} &= -\langle (C^A_{nm} - \langle C^A_{nm}\rangle_{AV})\, (C^B_{n'm'} - \langle C^B_{n'm'}\rangle_{AV})\rangle_{AV}, \\ \frac{\partial^2 A}{\partial \hat{\lambda}^A_{nm} \partial \lambda^B_{n'm'}} &= -\langle (\hat{C}^A_{nm} - \langle \hat{C}^A_{nm}\rangle_{AV})\, (C^B_{n'm'} - \langle C^B_{n'm'})\rangle_{AV})\rangle_{AV}, \\ \frac{\partial^2 A}{\partial \hat{\lambda}^A_{nm} \partial \hat{\lambda}^B_{n'm'}} &= -\langle (\hat{C}^A_{nm} - \langle \hat{C}^A_{nm}\rangle_{AV})\, (\hat{C}^B_{n'm'} - \langle \hat{C}^B_{n'm'})\rangle_{AV})\rangle_{AV}. \end{aligned} \tag{3.14}$$

Finally, we differentiate (3.8) with respect to λ^A_{nm} and $\hat\lambda^A_{nm}$ to obtain

$$\frac{\partial^2 A}{\partial\tau\partial\lambda^A_{nm}} = \langle(\mathbf{H} - \langle\mathbf{H}\rangle_{AV})(C^A_{nm} - \langle C^A_{nm}\rangle_{AV})\rangle_{AV} \tag{3.15}$$

and

$$\frac{\partial^2 A}{\partial\tau\partial\hat\lambda^A_{nm}} = \langle(\mathbf{H} - \langle\mathbf{H}\rangle_{AV})(\hat C^A_{nm} - \langle \hat C^A_{nm}\rangle_{AV})\rangle_{AV}, \tag{3.16}$$

as well as the corresponding identity with coefficient $\hat{\mathbf{H}} - \langle\hat{\mathbf{H}}\rangle_{AV}$ to obtain

$$\frac{\partial^2 A}{\partial\hat\tau\partial\lambda^A_{nm}} = \langle(\hat{\mathbf{H}} - \langle\hat{\mathbf{H}}\rangle_{AV})(C^A_{nm} - \langle C^A_{nm}\rangle_{AV})\rangle_{AV} \tag{3.17}$$

and

$$\frac{\partial^2 A}{\partial\hat\tau\partial\hat\lambda^A_{nm}} = \langle(\hat{\mathbf{H}} - \langle\hat{\mathbf{H}}\rangle_{AV})(\hat C^A_{nm} - \langle \hat C^A_{nm})\rangle_{AV})\rangle_{AV}. \tag{3.18}$$

Combining (3.3)-(3.18), we find that the Taylor expansion of A through second derivatives is given by

$$\begin{aligned}
&A(\tau+\delta\tau, \hat\tau+\delta\hat\tau, \tilde\lambda+\delta\tilde\lambda, \hat{\tilde\lambda}+\delta\hat{\tilde\lambda}\\
=&A(\tau,\hat\tau,\tilde\lambda,\hat{\tilde\lambda}) + \delta\tau\langle\mathbf{H}\rangle_{AV} + \delta\hat\tau\langle\hat{\mathbf{H}}\rangle_{AV} - \sum_{n\leq m,A}(\delta\lambda^A_{nm}\langle C^A_{nm}\rangle_{AV} + \delta\hat\lambda^A_{nm}\langle\hat C^A_{nm}\rangle_{AV})\\
-&\frac{1}{2}\langle[\delta\tau(\mathbf{H} - \langle\mathbf{H}\rangle_{AV}) + \delta\hat\tau(\hat{\mathbf{H}} - \langle\hat{\mathbf{H}}\rangle_{AV})\\
-&\sum_{m\leq n,A}\delta\lambda^A_{nm}(C^A_{nm} - \langle C^A_{nm}\rangle_{AV}) + \delta\hat\lambda^A_{nm}(\hat C^A_{nm} - \langle\hat C^A_{nm}\rangle_{AV})]^2\rangle_{AV};
\end{aligned} \tag{3.19}$$

the uniform negative sign of the quadratic term in the expansion indicates that A is a locally convex function, and shows that the matrix of second derivatives of A is negative semidefinite.

We now turn to the alternative expression of (2.21) for the partition function, defined in terms of an integral over the parameters of a sequence of microcanonical ensembles. The existence of a maximum in the integrand which dominates the integration assures the stability of the canonical ensemble; we now show that (3.19) implies the self-consistency of our assumption of a maximum.

Returning to (2.21), we see that the conditions for a maximum of the integrand at $\xi = \bar\xi$ are that there be a stationary point, i.e., that

$$\begin{aligned}
\tau =& \frac{\partial}{\partial E}S_{mic}(\xi)|_{\bar\xi},\\
\hat\tau =& \frac{\partial}{\partial \hat E}S_{mic}(\xi)|_{\bar\xi},\\
\lambda^A_{nm} =& -\frac{\partial}{\partial \nu^A_{nm}}S_{mic}(\xi)|_{\bar\xi},\\
\hat\lambda^A_{nm} =& -\frac{\partial}{\partial \hat\nu^A_{nm}}S_{mic}(\xi)|_{\bar\xi},
\end{aligned} \tag{3.20}$$

together with the requirement that the integrand should decrease in all directions, so that this point corresponds to a maximum. To make our demonstration of stability more transparent, let us define

$$\chi = \{\chi_i\} = \{\tau, \hat{\tau}, -\lambda^A_{nm}, -\hat{\lambda}^A_{nm}\}, \tag{3.21}$$

so that (3.20) takes the form

$$\chi_i = \frac{\partial S_{mic}}{\partial \xi_i}|_{\bar{\xi}}, \tag{3.22}$$

where the indices i are in the correspondence implied by (3.20), together with the requirement that the second derivative matrix

$$\frac{\partial^2 S_{mic}}{\partial \xi_i \partial \xi_j} = \frac{\partial \chi_i}{\partial \xi_j} \tag{3.23}$$

should be positive definite. But the values of E, $\hat{E}$, ν^A_{nm} and $\hat{\nu}^A_{nm}$ are equal to $\mathbf{H}$, $\hat{\mathbf{H}}$, C^A_{nm} and $\hat{C}^A_{nm}$ in the microcanonical ensemble, as seen from (2.3). If the stationary values are those given by $(3.3-4)$ and $(3.6-7)$, then we must have

$$\xi_i = \frac{\partial A}{\partial \chi_i}, \tag{3.24}$$

which implies that the matrix inverse to the right hand side of (3.23) is given by

$$\frac{\partial \xi_j}{\partial \chi_i} = \frac{\partial^2 A}{\partial \chi_i \partial \chi_j}, \tag{3.25}$$

which we have shown to be a negative semidefinite matrix. This in turn implies that the matrix on the right hand side of (3.23) is negative definite, giving the condition needed to assure that the stationary point in (3.20) is indeed a maximum.

Assuming this maximum dominates the integration, then the logarithm of the integral in (2.21) (up to an additive term which is relatively small for a large number of degrees of freedom) may be approximated by

$$A \cong \tau E + \hat{\tau}\hat{E} + \mathbf{Tr}\tilde{\lambda}\tilde{C} + \hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}} - S_{mic}(E,\, \hat{E}, \tilde{C},\, \hat{\tilde{C}}), \tag{3.26}$$

where the arguments are at the extremal values, giving the analog of the standard thermodynamical result $A = E - TS$ for the free energy.

4. The operators $\tilde{C}, \hat{\tilde{C}}$ as generators

The microcanonical ensemble is constructed as a set of elements of $\mathcal{S}$, which satisfy a constraint described by the value of $\mathbf{H}$. This subset of $\mathcal{S}$ is invariant to the flow generated by $\mathbf{H}$, where we define the flow induced by a functional according to the canonical transformation formulas of (1.10a) and (1.10b). As we have remarked above, the space is further restricted by values of $\hat{\mathbf{H}}$ and, in the canonical ensemble, the values of $\mathbf{Tr}\tilde{\lambda}\tilde{C}$ and

$\hat{\mathbf{Tr}}\hat{\tilde{\lambda}}\hat{\tilde{C}}$. Since these four quantities have vanishing Poisson brackets with each other under our present assumptions, the flow generated by all of these functionals lies in the constrained subset of $\mathcal{S}$. In constructing the microcanonical ensemble, we constrain the values of the conserved operators $\tilde{C}, \hat{\tilde{C}}$, i.e., we constrain the values of all total trace functionals constructed by projection from these operators. It is therefore instructive to study the action of general total trace functionals projected from $\tilde{C}$ and $\hat{\tilde{C}}$ as generators of canonical transformations on the phase space.

We first remark that it was pointed out in ref. 9 that a canonical generator of unitary transformations on the basis of the underlying Hilbert space has the form

$$\mathbf{G}_{\tilde{f}} = -\mathbf{Tr} \sum_r [\tilde{f}, p_r] q_r, \tag{4.1}$$

where $\tilde{f}$ is bosonic. Using (1.11) and the cyclic properties of $\mathbf{Tr}$, one sees that

$$\begin{aligned} \mathbf{G}_{\tilde{f}} &= -\mathbf{Tr} \tilde{f} \sum_r (p_r q_r - \epsilon_r q_r p_r) \\ &= \mathbf{Tr} \tilde{f} \tilde{C}. \end{aligned} \tag{4.2}$$

We thus see that the conserved operator $\tilde{C}$ has the additional role of inducing the action of unitary transformations on the underlying Hilbert space.

That this action preserves the algebraic properties of functionals of the type $\mathbf{G}_{\tilde{f}}$ can be seen by computing the Poisson bracket,

$$\{\mathbf{G}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} = \mathbf{Tr} \sum_r \epsilon_r \Big(\frac{\delta \mathbf{G}_{\tilde{f}}}{\delta q_r} \frac{\delta \mathbf{G}_{\tilde{g}}}{\delta p_r} - \frac{\delta \mathbf{G}_{\tilde{g}}}{\delta q_r} \frac{\delta \mathbf{G}_{\tilde{f}}}{\delta p_r} \Big). \tag{4.3a}$$

We use the result that

$$\begin{aligned} \delta \mathbf{G}_{\tilde{f}} &= \mathbf{Tr} \tilde{f} \delta \tilde{C} \\ &= \mathbf{Tr} \sum_r \{ \epsilon_r (\tilde{f} q_r - q_r \tilde{f}) \delta p_r - (\tilde{f} p_r - p_r \tilde{f}) \delta q_r \} \end{aligned} \tag{4.3b}$$

to obtain

$$\begin{aligned} \frac{\delta \mathbf{G}_{\tilde{f}}}{\delta q_r} &= -[\tilde{f}, p_r], \\ \frac{\delta \mathbf{G}_{\tilde{f}}}{\delta p_r} &= \epsilon_r [\tilde{f}, q_r], \end{aligned} \tag{4.4}$$

and hence, expanding out the commutators,

$$\begin{aligned} \{\mathbf{G}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} = -\mathbf{Tr} \sum_r \{ & p_r \tilde{f} q_r \tilde{g} - p_r \tilde{f} \tilde{g} q_r - \tilde{f} p_r q_r \tilde{g} + \tilde{f} p_r \tilde{g} q_r \\ & - p_r \tilde{g} q_r \tilde{f} + p_r \tilde{g} \tilde{f} q_r + \tilde{g} p_r q_r \tilde{f} - \tilde{g} p_r \tilde{f} q_r \}. \end{aligned} \tag{4.5}$$

The first and last terms on the right cancel under the **Tr**, as do the fourth and fifth. These cancellations do not depend on the grading under the trace, since they involve only cycling of the bosonic operators $\tilde{f}, \tilde{g}$. The remaining terms can be rearranged to the form

$$\begin{aligned} \{\mathbf{G}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} &= -\mathbf{Tr} \sum_r [\tilde{f}, \tilde{g}](p_r q_r - \epsilon_r q_r p_r) \\ &= \mathbf{Tr}[\tilde{f}, \tilde{g}]\tilde{C} \\ &= \mathbf{G}_{[\tilde{f}, \tilde{g}]}. \end{aligned} \tag{4.6}$$

These relations, corresponding to the group properties of integrated charges in quantum field theory, can be generalized to a "local" algebra. Defining

$$\mathbf{G}_{\tilde{f}r} = \mathbf{Tr} \tilde{f} \tilde{C}_r, \tag{4.7a}$$

where

$$\tilde{C}_r = \epsilon_r q_r p_r - p_r q_r, \tag{4.7b}$$

one obtains in the same way that

$$\{\mathbf{G}_{\tilde{f}r}, \mathbf{G}_{\tilde{g}s}\} = \delta_{rs} \mathbf{G}_{[\tilde{f}, \tilde{g}]r}. \tag{4.8}$$

In studying the flows induced by conserved operators, we shall also need the properties of generators projected from $\hat{\tilde{C}}$. We therefore define$^\diamond$

$$\hat{\mathbf{G}}_{\tilde{f}} = \mathbf{Tr} \tilde{f} \hat{\tilde{C}}. \tag{4.9}$$

Substituting (1.12), we find that the operator derivatives of $\hat{\mathbf{G}}_{\tilde{f}}$ with respect to the phase space variables are

$$\begin{aligned} \frac{\delta}{\delta q_r} \hat{\mathbf{G}}_{\tilde{f}} &= -(-1)^F [(-1)^F \tilde{f}, p_r] = -(\tilde{f} p_r - \epsilon_r p_r \tilde{f}), \\ \frac{\delta}{\delta p_r} \hat{\mathbf{G}}_{\tilde{f}} &= (-1)^F [(-1)^F \tilde{f}, q_r] = \tilde{f} q_r - \epsilon_r q_r \tilde{f}. \end{aligned} \tag{4.10}$$

Computing Poisson brackets in the same way as above, we find that the algebra of the generators $\mathbf{G}_{\tilde{f}}$ and $\hat{\mathbf{G}}_{\tilde{f}}$ closes,

$$\begin{aligned} \{\hat{\mathbf{G}}_{\tilde{f}}, \hat{\mathbf{G}}_{\tilde{g}}\} =& \mathbf{G}_{[\tilde{f}, \tilde{g}]}, \\ \{\hat{\mathbf{G}}_{\tilde{f}}, \mathbf{G}_{\tilde{g}}\} =& \{\mathbf{G}_{\tilde{f}}, \hat{\mathbf{G}}_{\tilde{g}}\} = \hat{\mathbf{G}}_{[\tilde{f}, \tilde{g}]}, \end{aligned} \tag{4.11}$$

$^\diamond$ In terms of this definition,

$$\hat{\mathbf{Tr}} \hat{\tilde{\lambda}} \hat{\tilde{C}} = \mathbf{Tr} (-1)^F \hat{\tilde{\lambda}} \hat{\tilde{C}} = \mathbf{G}_{(-1)^F \hat{\tilde{\lambda}}}.$$

giving a structure reminiscent of the vector and axial-vector charge algebra in quantum field theory. Just as the vector and axial-vector charge algebra can be diagonalized into two independent chiral charge algebras, so the algebra of (4.6) and (4.11) can be diagonalized into two independent algebras

$$\mathbf{G}_{\pm\tilde{f}} = \frac{1}{2}(\mathbf{G}_{\tilde{f}} \pm \hat{\mathbf{G}}_{\tilde{f}}), \tag{4.12}$$

which obey the algebra

$$\begin{aligned}\{\mathbf{G}_{\pm\tilde{f}}, \mathbf{G}_{\pm\tilde{g}}\} =& \mathbf{G}_{\pm[\tilde{f},\tilde{g}]}, \\ \{\mathbf{G}_{+\tilde{f}}, \mathbf{G}_{-\tilde{g}}\} =& 0.\end{aligned} \tag{4.13}$$

Defining a "local" version of $\hat{\mathbf{G}}_{\tilde{f}}$ by

$$\hat{\mathbf{G}}_{\tilde{f}r} = \mathbf{Tr}\tilde{f}\hat{\tilde{C}}_r, \tag{4.14}$$

where

$$\hat{\tilde{C}}_r = q_r p_r - p_r q_r, \tag{4.15}$$

the algebras of (4.11) and (4.13) can be converted to local versions analogous to (4.8).

We now turn to the flows associated with $\mathbf{G}_{\tilde{f}}$ and $\hat{\mathbf{G}}_{\tilde{f}}$ when used as canonical generators. Beginning with $\mathbf{G}_{\tilde{f}}$, we consider its action on the functional $\mathbf{x}_s(\eta)$ defined in (1.9a), for which $\delta\mathbf{x}_s(\eta) = \mathbf{Tr}\eta\delta x_s$. Defining a parameter γ along the motion generated by $\mathbf{G}_{\tilde{f}}$, we choose δx_s as $dx_s/d\gamma$, so that by (1.10a) we have

$$d\mathbf{x}_s(\eta) = \{\mathbf{x}_s(\eta), \mathbf{G}_{\tilde{f}}\}d\gamma. \tag{4.16}$$

Comparing (1.10b) with (4.4) and (4.16) gives

$$\begin{aligned}\frac{dq_s}{d\gamma} &= [\tilde{f}, q_s], \\ \frac{dp_s}{d\gamma} &= [\tilde{f}, p_s].\end{aligned} \tag{4.17}$$

In both the boson and fermion sectors we see that, as a solution of the differential equations (4.17), $\mathbf{G}_{\tilde{f}}$ induces the action of a unitary group generated by $\tilde{f}$,

$$x_s(\gamma) = e^{\tilde{f}\gamma} x_s(0) e^{-\tilde{f}\gamma}. \tag{4.18}$$

The unitary transformation (4.18) preserves the supremum operator norm

$$||x_s|| = \sup_{\{|n\rangle\}} \frac{|\langle n|x_s|n\rangle|}{|\langle n|n\rangle|}, \tag{4.19}$$

where the supremum is taken over all states $|n\rangle$ in Hilbert space. *

We next consider the canonical transformation induced on $\mathbf{x}_s(\eta)$ by the functional $\hat{\mathbf{G}}_{\tilde{f}}$ defined in (4.9). Introducing a parameter $\hat{\gamma}$ along the motion generated by $\hat{\mathbf{G}}_{\tilde{f}}$, we have in this case by (1.10a),

$$d\mathbf{x}_s(\eta) = \{\mathbf{x}_s(\eta), \hat{\mathbf{G}}_{\tilde{f}}\} d\hat{\gamma}. \tag{4.20}$$

Comparing (1.10b) with (4.10) and (4.20) gives

$$\begin{aligned} \frac{dq_s}{d\hat{\gamma}} &= \epsilon_s (-1)^F [(-1)^F \tilde{f}, q_s] = \epsilon_s \tilde{f} q_s - q_s \tilde{f}, \\ \frac{dp_s}{d\hat{\gamma}} &= (-1)^F [(-1)^F \tilde{f}, p_s] = \tilde{f} p_s - \epsilon_s p_s \tilde{f}. \end{aligned} \tag{4.21}$$

For the bosonic sector, (4.21) can be rewritten as

$$\begin{aligned} \frac{dq_s}{d\hat{\gamma}} =& [\tilde{f}, q_s], \\ \frac{dp_s}{d\hat{\gamma}} =& [\tilde{f}, p_s], \end{aligned} \tag{4.22}$$

and can be integrated as a unitary transformation for both q_s and p_s,

$$x_s(\hat{\gamma}) = e^{\tilde{f}\hat{\gamma}} x_s(0) e^{-\tilde{f}\hat{\gamma}}. \tag{4.23}$$

For the fermionic sector, however, the grading index $(-1)^F$ anticommutes with q_s and p_s and $\epsilon_s = -1$; consequently, the differential equations (4.21) in this case take the form

$$\begin{aligned} \frac{dq_s}{d\hat{\gamma}} &= -\{\tilde{f}, q_s\}, \\ \frac{dp_s}{d\hat{\gamma}} &= \{\tilde{f}, p_s\}, \end{aligned} \tag{4.24}$$

and involve *anticommutators* with the operator $\tilde{f}$, i.e., a graded action. We note, however, that the total trace Lagrangians for which $\hat{\tilde{C}}$ is conserved are ones in which the fermion fields appear as bosonic bilinears of the form $p_r q_s$; for these bilinears, and for the reverse ordered bosonic bilinears $q_s p_r$, we find from (4.24) that

$$\begin{aligned} \frac{d(p_r q_s)}{d\hat{\gamma}} &= [\tilde{f}, p_r q_s], \\ \frac{d(q_s p_r)}{d\hat{\gamma}} &= -[\tilde{f}, q_s p_r]. \end{aligned} \tag{4.25}$$

* The spectrum of x_s may be unbounded; the argument we have given above then applies to all bounded functions of the x_s, for which the operator norm exists. There is, moreover, a possibility that in the unbounded case, a phase space operator may be an eigenfunction of $\tilde{f}$, in the sense that $[\tilde{f}, x_s] = \sigma_s x_s$ for some real σ_s. The transformation (4.17) would then correspond to dilation, therefore admitting conformal transformations on some subset of the phase space $\mathcal{S}$ (for which preservation of the operator norm does not form an obstacle).

The solution of these differential equations is the unitary group action

$$\begin{aligned}(p_r q_s)(\hat{\gamma}) &= e^{\tilde{f}\hat{\gamma}}(p_r q_s)(0)e^{-\tilde{f}\hat{\gamma}},\\ (q_s p_r)(\hat{\gamma}) &= e^{-\tilde{f}\hat{\gamma}}(q_s p_r)(0)e^{\tilde{f}\hat{\gamma}},\end{aligned} \tag{4.26}$$

which preserves the supremum operator norm of the bilinears $p_r q_s$ and $q_s p_r$. However, it is easy to see that for fermionic operators, the supremum operator norm of (4.19) is not preserved by the evolution of (4.24) .†

Finally, it is also useful to define parameters $\gamma_{\pm}$ along the flows generated by $\mathbf{G}_{\pm\tilde{f}}$ according to

$$d\mathbf{x}_s(\eta) = \{\mathbf{x}_s(\eta), \mathbf{G}_{\pm\tilde{f}}\}d\gamma_{\pm}, \tag{4.27a}$$

so that

$$\frac{dx_s}{d\gamma_{\pm}} = \frac{1}{2}\left(\frac{dx_s}{d\gamma} \pm \frac{dx_s}{d\hat{\gamma}}\right). \tag{4.27b}$$

Then taking sums and differences of (4.17) and (4.22), (4.24) we find that for bosons (with x_s either q_s or p_s),

$$\begin{aligned}\frac{dx_s}{d\gamma_+} =&[\tilde{f}, x_s],\\ \frac{dx_s}{d\gamma_-} =&0,\end{aligned} \tag{4.28a}$$

which integrate to

$$\begin{aligned}x_s(\gamma_+) =&e^{\tilde{f}\gamma}x_s(0)e^{-\tilde{f}\gamma},\\ x_s(\gamma_-) =&x_s(0).\end{aligned} \tag{4.28b}$$

Similarly, for fermions we find that

$$\begin{aligned}\frac{dq_s}{d\gamma_+} &= -\,q_s\tilde{f}\ , \quad \frac{dp_s}{d\gamma_+} = \tilde{f}\ p_s,\\ \frac{dq_s}{d\gamma_-} &=\tilde{f}\ q_s\ , \qquad \frac{dp_s}{d\gamma_-} = -p_s\tilde{f},\end{aligned} \tag{4.29a}$$

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† For example, to lowest order in $\delta\hat{\gamma}$, for the fermionic coordinate variable q_s we have

$$(n, q_s(\delta\hat{\gamma})n) = (n, q_s n) - [(n, \tilde{f}q_s n) + (n, q_s\tilde{f}n)]\delta\hat{\gamma} + O((\delta\hat{\gamma})^2).$$

Now, letting $n = g + h\delta\hat{\gamma}$, we obtain

$$\begin{aligned}(n, q_s(\delta\hat{\gamma})n) = (g, q_s g) &+ [(h, q_s g) + (g, q_s h)]\delta\hat{\gamma}\\ &- [(g, \tilde{f}q_s g) + (g, q_s\tilde{f}g)]\delta\hat{\gamma} + O((\delta\hat{\gamma})^2).\end{aligned}$$

Taking $h = \tilde{f}g$, we see that $(g, q_s h) = (g, q_s\tilde{f}g)$ cancels the fifth term on the right, but $(h, q_s g) = (\tilde{f}g, q_s g) = -(g, \tilde{f}q_s g)$ does not cancel the fourth. The action of the diagonalized generators defined in (4.12) is therefore norm preserving on bosonic, but not on fermionic operators.

which integrate to

$$\begin{aligned} q_s(\gamma_+) =& q_s(0)e^{-\tilde{f}\gamma_+} \ , \quad p_s(\gamma_+) = e^{\tilde{f}\gamma_+}p_s(0), \\ q_s(\gamma_-) =& e^{\tilde{f}\gamma_-}q_s(0) \ , \quad\ \ p_s(\gamma_-) = p_s(0)e^{-\tilde{f}\gamma_-} . \end{aligned} \tag{4.29b}$$

This identifies $\mathbf{G}_{\pm\tilde{f}}$ as the generators of the one-sided unitary transformations acting on the fermions which are discussed in refs. 1 and 2.

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